PROTON EXCHANGE MEMBRANE FUEL CELLS: MODELING AND SIMULATION USING ADAPTIVE FINITE ELEMENTS

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Proton Exchange Membrane (PEM) Fuel Cells are the most promising of the current fuel cell technologies for efficiently producing zero–emission energy in a variety of mobile and stationary applications. The problem is challenging because of the coupling of eletrochemical reactions with transport phenomena, including multicomponent gas flow, two–phase flow, heat and mass transfer, phase change and transport of charge. An integral part of the extensive research into PEM fuel cells has been computational modeling and simulation [1–3] using either uniform grids or a priori graded meshes.

We focus on two main nonlinear components of the PEM fuel cell model: the multicomponent Stefan–Maxwell diffusion operator and the catalytic electrochemical reactions, given by the Butler–Volmer kinetics. Our computational approach uses adaptive, locally refined grids to resolve the solution features within the porous gas diffusers, the catalyst layers, and the membrane. These features include boundary layers and singularities arising from domain and boundary condition irregularities as well as nonlinear interactions [4]. A key component is an appropriate local error indicator for the element contribution to the global error, which provides accurate error estimation and guides the adaptive refinement process.

We present new local error indicators that are tailored to the types of nonlinear transport and reaction processes found in PEM fuel cells and more general reactive transport systems. Because residual—based error indicators are only rigorously justified for linear equations, we construct new local error indicators that incorporate the nonlinear character of the equation either by solving local nonlinear problems for the error or by appropriately weighting the local residual.

Numerical results are presented for transport of mass and charge in the porous electrode, catalyst layer, and membrane of a PEM fuel cell. A pseudo–arclength continuation algorithm is used to compute parameterized solution curves.

References

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